# Percolation properties of the 2D Heisenberg model

B. Allés[a], J. J. Alonso[b], C. Criado[b], M. Pepe[a]
[a] *Dipartimento di Fisica, Università di Milano-Bicocca and INFN Sezione di Milano, Milano, Italy*
[b] *Departamento de Física Aplicada I, Facultad de Ciencias, 29071 Málaga, Spain*

*Abstract*

We analyze the percolation properties of certain clusters defined on configurations of the 2–dimensional Heisenberg model. We find that, given any direction $\vec{n}$, in $O(3)$ space, the spins almost perpendicular to $\vec{n}$ form a percolating cluster. This result gives indications of how the model can avoid a previously conjectured Kosterlitz–Thouless phase transition at finite temperature $T$.

64.60.Cn; 05.50.+q; 75.10.Hk



The classical Heisenberg model in 2 dimensions (2D) describes the behaviour of a system of classical spins with short range ferromagnetic interactions [1]. The spins are placed at the sites of a 2D lattice. The physics of the model, which has been studied both through analytical calculations and Monte Carlo simulations, is defined by equations that display a continuous $O(3)$ symmetry and it is subject to the Mermin and Wagner theorem [2], i.e.: there are no equilibrium states with broken symmetry.

Perturbation theory (PT) indicates that the 2D Heisenberg model has a critical point at zero temperature [3]. Moreover, from the field–theoretical point of view, the spin field carries a particle of non–zero mass $m$. This mass has been calculated by applying a Bethe ansatz technique [4] and by making a partial use of PT. However, PT is constructed by studying small oscillations around the trivial configuration (all spins parallel), a state which obviously violates the Mermin and Wagner theorem. Therefore a problem raises concerning the validity of the above–mentioned analytical results and any other which relies on PT.

The model has also been studied by numerical simulations. Among other quantities (see for example [5]), the mass $m$ and the magnetic susceptibility $\chi$ have been recently measured with good precision. The mass is evaluated from the exponential decay of the 2–point correlation function $G(x-x')$. The magnetic susceptibility is extracted from the sum $\chi \equiv \sum_x G(x-x')$. Some of the most recent numerical calculations are the following. In [6,7] $m$ has been determined by extrapolating the result from small lattice sizes and large temperatures to smaller temperatures by using finite–size scaling. In [8] it has been extracted from the 2–point function by using improved actions and very high statistics. In both cases agreement with the analytical calculation of $m$ [4] is found within 2–4%.

Another scenario for the 2D Heisenberg model has been put forward in [9–11]. The model would undergo a Kosterlitz–Thouless (KT) phase transition at a finite temperature $T_{KT}$ and no massive particle would be carried by the spin field in the low temperature phase. This scenario is a mimic of what is known to happen in the 2D $O(2)$ or XY model [12]. If $T_{KT}$ is low enough, a numerical simulation is not able to detect it (in [8,13] it was argued that $T_{KT}$ is indeed much smaller than the typical temperatures utilized for thermalization in present–day simulations). In [14] a finite–size analysis of the helicity modulus is used to rule out such a KT transition for $T > 0.1$. In [8,13] it was also shown that the data for the correlation length and the magnetic susceptibility for temperatures $T > 0.53$ do not scale as the KT scenario predicts.

In the present paper, we want to tackle directly the arguments of [10,11] where the percolation properties of certain clusters are analyzed and, after assuming a set of hypotheses, it is concluded that the magnetic susceptibility diverges which is sufficient to prove that the mass $m$ vanishes.

We realize the classical spins of the Heisenberg model by 3–component scalar fields of modulus 1 placed at each site $x$ of a square lattice, $\vec{\phi}_x$ with $\left(\vec{\phi}_x\right)^2 = 1$. These fields interact through a nearest neighbour (n.n.) coupling and the hamiltonian can be written as ($\langle x\, y\rangle$ stands for two generic n.n. sites)

$$H \equiv \sum_{\langle x\, y\rangle} \vec{\phi}_x \cdot \vec{\phi}_y \ . \tag{1}$$

The partition function at a temperature $T$ is $Z = \sum_{\{\vec{\phi}_x\}} \exp\left(H/T\right)$. The hamiltonian (1) and the partition function are invariant under $O(3)$ rotations.

In the following we recall the arguments of [10,11]. Let us consider a configuration for this model thermalized at a given temperature $T$. Let $\vec{n}$ be an arbitrary unit vector in the internal space of the $O(3)$ symmetry. To any such a vector we can associate various types of clusters on the configuration. If $\mathcal{A}$ is one such cluster then its size, defined as the number of sites contained in it, shall be denoted by $C_{\mathcal{A}}$. On the other hand, its perimeter, defined as the number of sites along the border of the cluster, will be called $B_{\mathcal{A}}$. If a set of clusters completely cover the whole lattice volume with no overlap then we say that we have a "cluster system".

The Fortuin–Kasteleyn clusters (hereafter called

$\mathcal{F}$) [15] are made of sites connected by the bonds which survive the deletion process performed with the probability

$$P_{xy} \equiv \exp\left(\min\{0\,,\,-\frac{2}{T}\left(\vec{\phi}_x\cdot\vec{n}\right)\left(\vec{\phi}_y\cdot\vec{n}\right)\}\right)\,. \qquad (2)$$

The average size of the $\mathcal{F}$ clusters satisfies $\langle C_{\mathcal{F}}\rangle = \kappa\,\chi$ where $\chi$ is the magnetic susceptibility and $\kappa$ is a constant $\kappa < 1$. The brackets $\langle\cdot\rangle$ indicate average over configurations or equivalently the average calculated with the Boltzmann weight of the partition function. In physical terms, $\mathcal{F}$ clusters are regions of correlated spins. The set of $\mathcal{F}$ clusters form a cluster system.

Other clusters associated to an arbitrary unit vector $\vec{n}$ are the $\mathcal{H}^+$, $\mathcal{H}^-$ and $\mathcal{S}$ clusters. All n.n. spins on a thermalized configuration at a temperature $T$ tipically satisfy $\|\vec{\phi}_x - \vec{\phi}_y\| \leq \varepsilon$ with a parameter $\varepsilon$ of order $O\left(\sqrt{2\,T}\right)$. Then for any site $x$ the scalar product $\left(\vec{\phi}_x\cdot\vec{n}\right)$ can be either *a)* $\left(\vec{\phi}_x\cdot\vec{n}\right) > \varepsilon/2$, and $x$ belongs to an $\mathcal{H}^+$ cluster, or *b)* $\left(\vec{\phi}_x\cdot\vec{n}\right) < -\varepsilon/2$, so $x$ belongs to an $\mathcal{H}^-$ cluster, or *c)* $|\vec{\phi}_x\cdot\vec{n}| \leq \varepsilon/2$ and consequently $x$ belongs to an $\mathcal{S}$ cluster. In simple words, the $\mathcal{S}$ clusters are constituted by sites whose spins almost lie in the plane perpendicular to $\vec{n}$; on the other hand the $\mathcal{H}^+$ ($\mathcal{H}^-$) clusters contain sites whose spins are almost parallel (antiparallel) to $\vec{n}$. The set of $\mathcal{H}^\pm$ and $\mathcal{S}$ clusters form a cluster system.

By using a variant of the $O(3)$ model that includes a Lipschitz continuity condition, $\|\vec{\phi}_x - \vec{\phi}_y\| \leq \delta$ for all n.n. $x$, $y$ (this condition does not change the physical properties of the model as long as $\delta > \varepsilon$), it is possible to prove that the $\mathcal{H}^\pm$ clusters lie entirely inside the $\mathcal{F}$ clusters [10,11]. Moreover no $\mathcal{H}^+$ cluster has a common frontier with any $\mathcal{H}^-$ cluster, they are always separated by spins belonging to $\mathcal{S}$ type clusters.

Following Ref. [10,11], three hypotheses are now necessary to prove that the magnetic susceptibility diverges. The first one states the impossibility to have simultaneous percolation of two or more disjoint clusters in a cluster system defined on the 2D Heisenberg model. This fact is known to be true in several models [16]. The second hypothesis extends the validity of the Mermin and Wagner theorem to hamiltonians which, like the one including the Lipschitz condition, are not differentiable in the fields. These two conditions altogether prevent the $\mathcal{H}^\pm$ clusters from percolating.

The third hypothesis is to assume that the $\mathcal{S}$ type clusters do not percolate either. Consequently none of the $\mathcal{H}^\pm$ or $\mathcal{S}$ clusters percolate. When a cluster system does not contain a percolating cluster then at least two kinds of clusters have a divergent average size [17]. In the cluster system of $\mathcal{H}^\pm$ and $\mathcal{S}$, this result means that either $\langle C_{\mathcal{H}^+}\rangle = \infty$ or $\langle C_{\mathcal{H}^-}\rangle = \infty$ or both (actually both, to avoid the breaking of the second hypothesis). Moreover, as the $\mathcal{H}^\pm$ clusters are entirely included inside the $\mathcal{F}$ clusters, these clusters must also have a divergent average size. Therefore the magnetic susceptibility $\chi$ diverges and the theory is massless in clear contrast to the calculation of [4].

The above conclusion can be avoided if at least one of the three hypotheses fails. In particular we have checked the third one finding that there does exist a $\mathcal{S}$ cluster which percolates. In the present paper we report the results of a numerical simulation of the Heisenberg model at $T = 0.5$ on very large lattices to give evidence that this is indeed the case at that temperature. We describe how this percolation takes place in the system, showing that a percolating $\mathcal{S}$ cluster is found for every direction $\vec{n}$ in the symmetry group space $O(3)$. Moreover all (percolating or not) $\mathcal{S}$ and $\mathcal{H}^\pm$ clusters present a high degree of roughness. More specifically, every spin in a cluster has on average one n.n. lying on the border of the cluster, (on a 2D square lattice each spin has four n.n.). In the following we describe the technical details of our simulation and give the results obtained.

We have simulated the system described by the hamiltonian in Eq.(1) on several lattice sizes $L^2$ with $L = 1024$, 1250, 1550 and 2048 at a temperature $T = 0.5$. The measurements and cluster analysis have been performed on a sample of between 1000 and 2000 configurations which were separated by 200 overheatbath updating steps [18], (this updating method applies a usual heatbath step to the dynamical variables –the angle formed by the spin field $\vec{\phi}_x$ and the sum of their n.n.– and fixes the other variables by maximizing the distance between the old and the new updated fields $\vec{\phi}_x$ in order to hasten the decorrelation).

The percolation of clusters is a well–defined concept on infinite lattices. Obvious computer limitations force us to work on finite volume systems. We have overcome this difficulty by working with a large ratio $L/\xi$ where $\xi$ is a typical correlation length of the system. In this way we expect that the would–be percolating cluster will show up as a very large cluster, much larger than the others. We have chosen our simulation parameters in such a way that $L/\xi \geq 4.5$, see Ref. [19].

The first task is to decide the value for $\varepsilon$ to be used in the construction of clusters. $\varepsilon$ should not be too large in order to avoid a certain (but not instructive for our problem) percolation of the $\mathcal{S}$ clusters, the estimate $\varepsilon \approx \sqrt{2\,T}$ being an appropriate value. In Fig. 1 we show the probability distribution of values of $\|\vec{\phi}_x - \vec{\phi}_y\|$ for all n.n. $x$, $y$ on a lattice of size $L = 1024$ at $T = 0.5$. The error bars in this and in the subsequent figures are very small: we show only the error bar of the data point on the top of Fig. 1. Motivated by this distribution we have taken $\varepsilon = 1.05$ which satisfies the estimate $\varepsilon \approx \sqrt{2\,T} = 1$. We have checked that, by using this value of $\varepsilon$, the $\mathcal{H}^+$ and $\mathcal{H}^-$ clusters touch each other only in a 0.5% of all bonds and this is shown in the inset of Fig. 1 where we give the fraction of bonds which join $\mathcal{H}^+$ and $\mathcal{H}^-$ clusters, $F_H$, as a function of $\varepsilon$. At $\varepsilon = 1.05$ we will already find evidence

for the existence of percolating $\mathcal{S}$ clusters. For smaller epsilons one cannot longer prove that the $\mathcal{H}^{\pm}$ clusters lie entirely inside the $\mathcal{F}$ clusters, which is an essential ingredient for the arguments given in [10,11]. We could choose smaller values of $\varepsilon$ only at lower temperatures.

We have taken several choices for the vector $\vec{n}$. In all cases we observed exactly the same results. In this paper we report the figures obtained with $\vec{n} = (1, 0, 0)$.

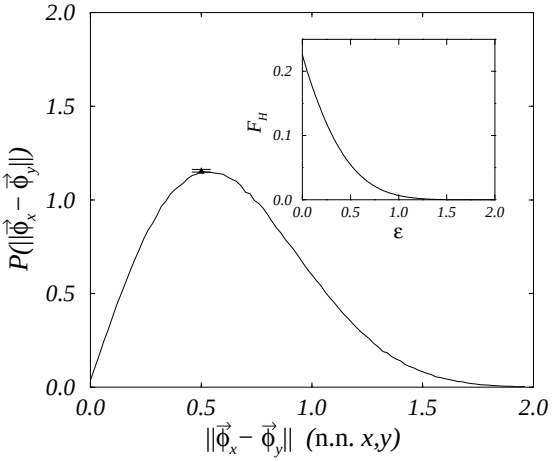


FIG. 1. Probability distribution of $\|\vec{\phi}_x - \vec{\phi}_y\|$ for all n.n. $x$, $y$ on a lattice of size $L = 1024$ at $T = 0.5$. In the inset: fraction of bonds that connect $\mathcal{H}^+$ and $\mathcal{H}^-$ sites as a function of $\varepsilon$.

In Fig. 2 we show the distribution of sizes for the three types of clusters, $\mathcal{S}$ (circles) and $\mathcal{H}^{\pm}$ (triangles). We present the data for each cluster size $C$ up to sizes $C = 100$; for larger values of $C$ we show the results averaged over bins $[\ln C - \eta/2, \ln C + \eta/2]$ with $\eta \approx 0.5$. The quantity $P(C)\,\mathrm{d}C$ is proportional to the probability of finding a cluster with size between $C$ and $C + \mathrm{d}C$. The line with triangles is continuous and it ends at $\ln C = 10.2$. On the other hand the curve with circles, which represents the $\mathcal{S}$ clusters, displays two parts: a continuous line ending at $\ln C = 9.2$ and a separated point at $\ln C \approx 13.1$. This isolated point is the one determined by the percolating cluster. Although not explicitely depicted, this point has an horizontal error bar which results in the slight horizontal spreading of circles. This error bar is a remnant of the fact that on truly infinite lattices the size of the percolating cluster must be infinite. Notice that the continuous part of the curve with circles becomes steeper just before ending at $\ln C = 9.2$: this is another indication for the existence of a percolating cluster [20] because it means that all clusters beyond some size prefer to be absorbed by the percolating $\mathcal{S}$ cluster. This figure has been obtained by working on a lattice size $L = 1024$ and choosing $\vec{n} = (1, 0, 0)$. Completely analogous results are obtained with other sizes $L$ and any other unit vector $\vec{n}$. We then conclude that there always exists a percolating cluster of type $\mathcal{S}$ for any versor $\vec{n}$.

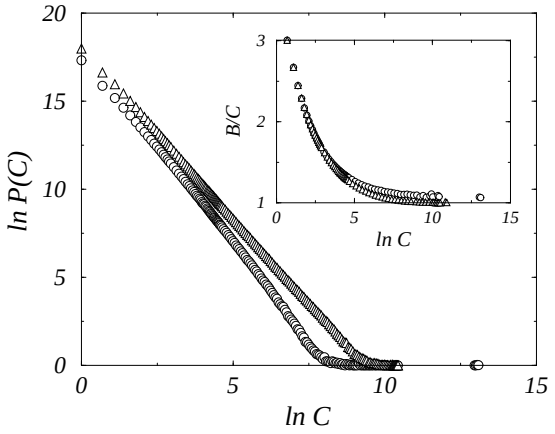


FIG. 2. Size distribution of $\mathcal{S}$ (circles) and $\mathcal{H}^{\pm}$ (triangles) clusters on $L = 1024$ at $T = 0.5$ and $\varepsilon = 1$ on a log–log scale. In the inset: ratio perimeter/size of clusters as a function of their size.

In Fig. 3 an example of a type $\mathcal{S}$ percolating cluster taken from a single thermalized configuration is shown. The percolating sites are coloured in black. To render the fine details of the clusters as clear as possible we show only a piece of size $512 \times 512$ taken out from a configuration on a lattice with $L = 1024$. The figure corresponds to the percolating cluster found in the plane perpendicular to $\vec{n} = (1, 0, 0)$. It is clear from this figure that the clusters present a high degree of roughness.

The property of roughness is made explicit in the inset of Fig. 2. The ratio "perimeter of cluster"/"size of cluster", $B/C$, is displayed against $\ln C$ for all $\mathcal{H}^{\pm}$ (triangles) and $\mathcal{S}$ (circles) clusters (irrespective of the fact that they percolate or not). For bidimensional compact objects $B/C \propto 1/\sqrt{C}$ when $C \to \infty$. In our case this ratio tends to a constant (which is almost 1) when $C \to \infty$ and this is an indicative that our clusters present a rough border, suggesting that they have a fractal structure.

In the inset of Fig. 2 we see that the ratio $B/C$ goes asymptotically to a constant which seems to be a bit larger for the $\mathcal{S}$ clusters than for $\mathcal{H}^{\pm}$. We think that this is because the $\mathcal{S}$ clusters surround the $\mathcal{H}^{\pm}$ clusters (see the introduction) and consequently they need to have an additional boundary.

We have also studied the ratio among the size of the largest (always percolating) $\mathcal{S}$ cluster, $M_{\mathcal{S}} \equiv \max\{C_{\mathcal{S}}\}$, and the size of the largest $\mathcal{H}^{\pm}$, $M_{\mathcal{H}} \equiv \max\{C_{\mathcal{H}^{\pm}}\}$, as a function of the lattice size $L$. Let us call $R$ such ratio,

$$R \equiv \frac{\langle M_{\mathcal{S}} \rangle}{\langle M_{\mathcal{H}} \rangle} \,. \tag{3}$$

If $R$ increases with $L$ for a fixed temperature, we can reasonably infer that the above described percolation properties survive the thermodynamic limit. The data for $R$ and the maximum size of $\mathcal{S}$ and $\mathcal{H}^{\pm}$ clusters are shown in Table 1 from the four lattice sizes we have used. They indicate that indeed the largest $\mathcal{S}$ cluster keeps percolating

when $L$ increases. Notice that the percentage of lattice volume covered by the percolating cluster does not vary appreciably with the lattice size $L$.

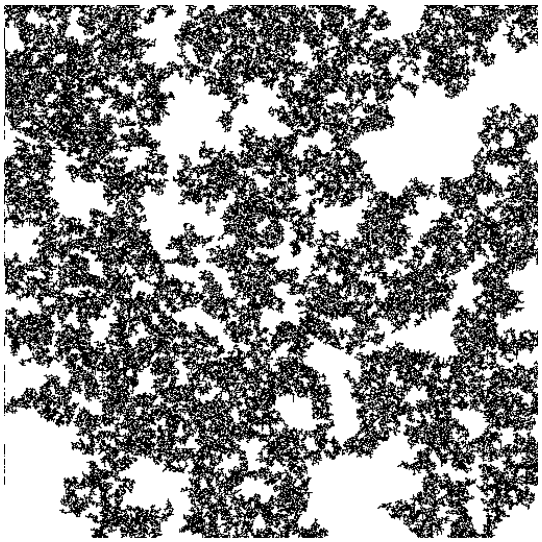

FIG. 3. Percolating $\mathcal{S}$ cluster (in black) from a thermalized configuration on a lattice of size $L = 1024$.

TABLE 1. Ratio $R$ and maximum sizes of clusters as a function of the lattice size $L$.

| $L$ | 1024 | 1250 | 1550 | 2048 |
|---|---|---|---|---|
| $\langle M_{\mathcal{S}} \rangle / L^2$ | 0.437(10) | 0.429(4) | 0.433(7) | 0.424(4) |
| $\langle M_{\mathcal{H}} \rangle / L^2$ | 0.019(3) | 0.015(2) | 0.011(1) | 0.0072(7) |
| $R$ | 23(4) | 29(4) | 40(4) | 59(6) |

In conclusion, we have studied the percolation properties of several clusters which can be defined on configurations of the 2D Heisenberg model described by the hamiltonian in Eq. (1). Of particular interest are the clusters called $\mathcal{S}$. To define them one has to introduce an arbitrary unit vector $\vec{n}$ in the symmetry group space of the system, $O(3)$. When the spin $\vec{\phi}_x$ at the site $x$ is almost perpendicular to $\vec{n}$, we say that this site belongs to some $\mathcal{S}$ cluster. The term "almost perpendicular" depends on the temperature $T$ of the system (see above). For $T = 0.5$ and working on rather large lattice sizes $L \geq 1024$, we have given strong evidence that for every $\vec{n}$ one of these $\mathcal{S}$ clusters percolates on each thermalized configuration of the system (see Fig. 2). These percolation properties seem to survive the thermodynamic limit (see Table 1).

This is an important conclusion because if such clusters do not percolate then one can prove [10,11] that the system carries no massive particle, contradicting the exact calculation of the mass gap performed for this theory in Ref. [4]. Our results exclude this massless phase for $T > 0.5$.

We have also shown that, at least at $T = 0.5$, all clusters present a high degree of roughness recalling a fractal structure, (see inset in Fig. 2 and Fig. 3). It seems unlikely that, as suggested in [10], such a dilute set of spins, almost lying on a plane, can enforce the system to behave like an effective $O(2)$ model (see [21]).

We wish to thank Andrea Pelissetto for discussions and Julio Fernández for a careful reading of the manuscript. B. A. also thanks the warm hospitality at the Departamento de Física Aplicada I of the Málaga University during the completion of the paper.

[1] E. Brézin and J. Zinn-Justin, Phys. Rev. B 14 (1976) 3110.
[2] N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17 (1966) 1133.
[3] A. M. Polyakov, Phys. Lett. B 59 (1975) 79.
[4] P. Hasenfratz, M. Maggiore and F. Niedermayer, Phys. Lett. B 245 (1990) 522.
[5] J. Balog *et al.*, hep-lat/9903036.
[6] J. K. Kim, Phys. Rev. Lett. 70 (1993) 1735.
[7] S. Caracciolo, R. G. Edwards, A. Pelissetto and A. D. Sokal, Phys. Rev. Lett. 75 (1995) 1891.
[8] B. Allés, A. Buonanno and G. Cella, Nucl. Phys. B 500 [FS] (1997) 513.
[9] H. E. Stanley and T. A. Kaplan, Phys. Rev. Lett. 17 (1966) 913; H. E. Stanley, Phys. Rev. Lett. 20 (1968) 150.
[10] A. Patrascioiu and E. Seiler, Nucl. Phys. B (Proc. Suppl.) 30 (1993) 184.
[11] A. Patrascioiu and E. Seiler, J. Stat. Phys. 69 (1992) 573.
[12] J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6 (1973) 1181.
[13] B. Allés, G. Cella, M. Dilaver and Y. Gündüç, Phys. Rev. D59 (1999), 067703.
[14] N. Schultka, Phys. Rev. B55 (1997) 41.
[15] C. M. Fortuin and P. W. Kasteleyn, Physica 57 (1972) 536.
[16] See [11] and references therein. Our formulation of this hypothesis is less general than the original one appearing in [11] but it is still enough for the purpose of the proof.
[17] For instance: A. Bunde and S. Havlin in *"Fractals and Disordered Systems"*, Springer–Verlag, Berlin, (1991).
[18] R. Petronzio and E. Vicari, Phys. Lett. B254 (1991) 444.
[19] J. Apostolakis, C. F. Baillie and G. C. Fox, Phys. Rev. D43 (1991) 2687.
[20] J. L. Cambier and M. Nauenberg, Phys. Rev. B34 (1986) 8071.
[21] T. Koma and H. Tasaki, Phys. Rev. Lett. 74 (1995) 3916; A. Vallat, S. E. Korshunov and H. Beck, Phys. Rev. B43 (1991) 8482.